

We claim:

1. A method for obtaining an improved estimate of a property useful in a chemical manufacturing process employing an on-line analyzer, the method comprising
5 the steps of:

mathematically transforming data obtained from an on-line analyzer to obtain scores correlative to the property; and

regressing the scores with one or more process variables to generate an estimate of the property.

10 2. The method of Claim 1 wherein the estimate is used in the control of a polyolefin reactor and the reactor is used to manufacture a polymeric material selected from the group consisting of polymers containing at least fifty weight percent of material originating as propylene monomer units, and polymers containing at least fifty weight percent of material originating as ethylene monomer units.

15 3. The method of Claim 1 wherein a nuclear magnetic resonance spectrometer is used to obtain free induction decay curve data which is mathematically transformed to obtain scores, and in which the scores are regressed with the one or more process variables for the purpose of estimating melt flow rate of the polymeric material.

20 4. The method of Claim 1 wherein the on-line analyzer is selected from the group consisting of nuclear magnetic resonance, near infrared, infrared, ultraviolet-visible, X-ray fluorescence, ultrasonic, and Raman spectrometers.

5. The method of Claim 1 wherein at least a portion of the chemical manufacturing process occurs in a chemical reactor.

25 6. The method of Claim 5 wherein the chemical reactor is selected from the group consisting of gas phase fluidized bed reactors, gas phase subfluidized bed reactors, stirred tank reactors, liquid pool reactors, gas loop reactors having one or more fluidization domains, and supercritical loop reactors.

30 7. The method of Claim 6 wherein the on-line analyzer is a nuclear magnetic resonance spectrometer, and the scores are obtained by mathematically transforming free induction decay curves from the spectrometer.

8. The method of Claim 5 wherein nuclear magnetic resonance spectrometer is used to obtain data which is mathematically transformed to obtain scores which are regressed with one or more process variables for the purpose of estimating a melt flow rate of a polymeric material.

9. The method of Claim 8 wherein the process employs a polyolefin reactor, and the polymeric material is selected from the group consisting of polymers containing at least fifty weight percent of material originating as propylene monomer units and polymers containing at least fifty weight percent of material originating as ethylene monomer units.

10. The method of Claim 9 wherein the polymeric material is an impact copolymer comprising polymerized propylene and ethylene monomer units.

11. The method of Claim 9 wherein the polymeric material comprises at least fifty weight percent of material originating as propylene monomer units and at least two weight percent of material originating as monomer units of an olefin other than propylene or an alpha olefin having four or more carbon atoms.

12. The method of Claim 9 wherein the polymeric material comprises at least fifty weight percent of material originating as ethylene monomer units and at least two weight percent of material originating as monomer units of propylene or an alpha olefin having four or more carbon atoms.

13. The process of Claim 1 wherein the regression is a non-linear regression.

14. The process of Claim 1 wherein the regression is a linear regression.

15. The process of Claim 1 wherein at least one of the at least one process variable is a reactor process variable selected from the group consisting of Al/Mg ratio, first reactor catalyst yield, second reactor incremental catalyst yield, first reactor offgas temperature, hydrogen to propylene ratio for the first reactor, hydrogen to propylene ratio for the second reactor, ethylene to propylene ratio for the second reactor, and percent rubber in a final impact copolymer product.

16. A chemical manufacturing process comprising the steps of:

using an on-line analyzer to collect data related to a chemical material at a point within the manufacturing process;

mathematically transforming the data to produce scores related to the chemical material;

regressing the scores with one or more process variables to produce an estimate of a property of interest for the chemical material; and

5 inputting the estimated property into a controller used in the chemical manufacturing process.

17. The process of Claim 16 further comprising the step of varying the output of the controller in response to the inputted estimated property to cause the property of interest to move toward a desired value.

10 18. The process of Claim 17 wherein the controller is selected from the group consisting of PID and fuzzy logic controllers.

19. The process of Claim 18 wherein there are at least two or more controllers selected from the group of PID controllers, fuzzy logic controllers, and combinations thereof.

15 20. The process of Claim 16 wherein the process includes a chemical reactor and one or more process variables are reactor process variables.

21. The process of Claim 20 wherein the chemical reactor is selected from the group consisting of gas phase fluidized bed reactors, gas phase subfluidized bed reactors, stirred tank reactors, liquid pool reactors, gas loop reactors having one or more
20 fluidization domains, and supercritical loop reactors.

22. The process of Claim 16 wherein the on-line analyzer is selected from the group consisting of nuclear magnetic resonance, near infrared, infrared, ultraviolet-visible, X-ray fluorescence, ultrasonic, and Raman spectrometers.

23. The process of Claim 16 wherein the data collected comprise free
25 induction decay curves obtained from a nuclear magnetic resonance spectrometer.

24. The process of Claim 23 wherein the property of interest is melt flow rate.

25. The process of Claim 21 wherein the data collected comprise free induction decay curves obtained from a nuclear magnetic resonance spectrometer, and wherein the property of interest is melt flow rate.

30 26. The process of Claim 20 wherein the process employs a polyolefin reactor to manufacture a polymeric material, and the polymeric material is selected from the

group consisting of polymers containing at least fifty weight percent of material originating as propylene monomer units and polymers containing at least fifty weight percent of material originating as ethylene monomer units.

27. The process of Claim 20 wherein the chemical manufactured in the
5 chemical manufacturing process comprises a polymeric chemical selected from the group consisting of terephthalic acid, polystyrene, polyethylene, polypropylene, polymers of alpha-olefin monomers containing from 4 to 20 carbon atoms, polyvinyl chloride, polyethylene terephthalate, and combinations thereof.